Cyclohexane, 1-methyl-2-propyl-

Other names: 1-Methyl-2-propylcyclohexane
Inchi: InChI=1S/C10H20/c1-3-6-10-8-5-4-7-9(10)2/h9-10H,3-8H2,1-2H3
InchiKey: BVYJEKBXVYKYRA-UHFFFAOYSA-N
Formula: C10H20
SMILES: CCCC1CCCCC1C
Mol. weight [g/mol]: 140.27
CAS: 4291-79-6

Physical Properties

Property code	Value	Unit	Source
gf	50.06	kJ/mol	Joback Method
hf	-215.75	kJ/mol	Joback Method
hfus	14.56	kJ/mol	Joback Method
hvap	37.97	kJ/mol	Joback Method
log10ws	-3.42		Crippen Method
logp	3.613		Crippen Method
mcvol	140.900	ml/mol	McGowan Method
pc	2485.07	kPa	Joback Method
rinpol	993.00		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	983.00		NIST Webbook
rinpol	983.00		NIST Webbook
tb	449.30 ± 3.00	K	NIST Webbook
tc	639.52	K	Joback Method
tf	205.60	K	Joback Method
vc	0.527	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.73	J/mol×K	443.08	Joback Method
cpg	389.89	J/mol×K	606.78	Joback Method
cpg	373.57	J/mol×K	574.04	Joback Method
cpg	356.42	J/mol×K	541.30	Joback Method

cpg	338.41	J/mol×K	508.56	Joback Method
cpg	319.51	J/mol×K	475.82	Joback Method
cpg	405.38	J/mol×K	639.52	Joback Method
dvisc	0.0002646	Pa×s	443.08	Joback Method
dvisc	0.0003397	Pa×s	403.50	Joback Method
dvisc	0.0004605	Pa×s	363.92	Joback Method
dvisc	0.0006724	Pa×s	324.34	Joback Method
dvisc	0.0010906	Pa×s	284.76	Joback Method
dvisc	0.0020679	Pa×s	245.18	Joback Method
dvisc	0.0050164	Pa×s	205.60	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.44169e+01
Coeff. B	-3.75566e+03
Coeff. C	-6.60140e+01
Temperature range (K), min.	331.82
Temperature range (K), max.	478.48

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4291796&Units=SI

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

gf: Standard Gibbs free energy of formation

hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume